Appendix D: Solving Elementary Parabolic Partial Differential Equations

The simplest equations of this type are often referred to as "conduction" or "diffusion" equations:

momentum	heat	mass	
$\frac{\partial V_x}{\partial t} = \nu \frac{\partial^2 V_x}{\partial y^2}$	$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial y^2}$	$\frac{\partial C_A}{\partial t} = D_{AB} \frac{\partial^2 C_A}{\partial y^2}$	(D1a,b,c)

We have numerous options in such cases, including: scaling or variable transformation, separation of variables, and a plethora of numerical methods. Let's consider the transformation of eq. (D1b) first; we define $\eta = \frac{y}{\sqrt{4\alpha t}}$, and write the left-hand side of (D1b) as

$$\frac{\partial T}{\partial \eta}\frac{\partial \eta}{\partial t} = T'\left(-\tfrac{1}{2}\right)\frac{y}{\sqrt{4\alpha}}t^{-3/2}. \tag{D2}$$

Differentiating the right-hand side of (D1b) the first time:

$$\frac{\partial T}{\partial \eta}\frac{\partial \eta}{\partial y} = T'\frac{1}{\sqrt{4\alpha t}}, \text{ and then again, we obtain: } T''\frac{1}{4\alpha t}. \tag{D3}$$

Substitution into (D1b) results in:

$$-2\eta\frac{dT}{d\eta} = \frac{d^2T}{d\eta^2}\ , \tag{D4}$$

an ordinary differential equation. Whether or not (D4) can produce a useful solution depends upon the nature of the problem. For transient conduction in an infinte slab, or viscous flow near a wall suddenly set in motion, it results in the familiar error function solution; e.g.,

$$\theta = 1 - erf\left(\frac{y}{\sqrt{4\alpha t}}\right). \tag{D5}$$

For contrast, let's now examine conduction in a *finite* slab of material; let this object extend from y=0 to y=1. We can have either a uniform initial temperature, or a temperature distribution that can be written as a function of y. At t=0, both faces are instantaneously heated to some new temperature, T_s. Define a dimensionless temperature,

$\theta = \frac{T - T_s}{T_i - T_s}$, and let θ=f(y)g(t). The product method yields

$$g' = -\alpha\lambda^2 g \qquad \text{and} \qquad f'' + \lambda^2 f = 0\,. \tag{D6}$$

As expected, we get

$$g = C_1 \exp(-\alpha\lambda^2 t) \qquad \text{and} \qquad f = A\sin\lambda y + B\cos\lambda y\,. \tag{D7}$$

Since B must be zero, and sin(λ)=0, we very quickly find

$$\theta = \sum_{n=1}^{\infty} A_n \exp(-\alpha\lambda_n{}^2 t)\sin\lambda_n y\,. \tag{D8}$$

If we have a uniform initial temperature, T_i, then application of the initial condition results in:

$$1 = \sum_{n=1}^{\infty} A_n \sin\lambda_n y\,, \tag{D9}$$

a half-range Fourier sine series. By theorem,

$$A_n = \frac{2}{L}\int_0^L f(y)\sin\frac{n\pi y}{L}\,dy\,, \tag{D10}$$

but for our case L=1 and the function, f(y), is also 1. The integral, (D10), is zero for even n and equal to 4/(nπ) for n=1,3,5,… With this example we have a good opportunity to examine the convergence of the infinite series solution. Let y=1/2, α=0.1, and let t range from 0.001 to 0.625 by repeated factors of 5. We'll examine the series for n's from 1 to 43; see Table D1. Note that for small t's the series does not converge quickly. However, for t=0.125 we need only five terms and at t=0.625, only three. The results should not be surprising. For very small t's, the temperature profile is virtually half a cycle of a square wave.

An Elementary, Explicit Numerical Procedure

Suppose we have viscous flow near a plane wall set in motion with velocity, V_0, at t=0. Letting $V=V_x/V_0$,

$$\frac{\partial V}{\partial t} = \nu\frac{\partial^2 V}{\partial y^2}\,. \tag{D11}$$

An explicit algorithm is easily developed for (D11):

$$V_{i,j+1} = \frac{\Delta t\,\nu}{(\Delta y)^2}\left[V_{i+1,j} - 2V_{i,j} + V_{i-1,j}\right] + V_{i,j}\,. \tag{D12}$$

Table D1. Illustration of infinite series convergence for small t's.

term no.	t=0.001	t=0.005	t=0.025	t=0.125	t=0.625
1	1.271981	1.266969	1.242205	1.12546	0.6870893
3	0.851322	0.8609938	0.9023096	0.9856378	0.6854422
5	1.099763	1.086086	1.039727	0.9972914	0.6854423
7	0.926459	0.9432634	0.9854355	0.9968604	0.6854423
9	1.05706	1.038121	1.004608	0.9968669	0.6854423
11	0.954341	0.9744126	0.9987616	0.9968669	0.6854423
13	1.037236	1.01695	1.000275	0.9968669	0.6854423
15	0.969256	0.9889856	0.9999457	0.9968669	0.6854423
17	1.025566	1.006978	1.000006	0.9968669	0.6854423
19	0.97864	0.9956936	0.9999966	0.9968669	0.6854423
21	1.017874	1.002573	0.9999977	0.9968669	0.6854423
23	0.985031	0.9985044	0.9999976	0.9968669	0.6854423
25	1.012515	1.000835	0.9999976	0.9968669	0.6854423
27	0.98955	0.9995433	0.9999976	0.9968669	0.6854423
29	1.008694	1.000235	0.9999976	0.9968669	0.6854423
31	0.992785	0.9998772	0.9999976	0.9968669	0.6854423
33	1.005956	1.000056	0.9999976	0.9968669	0.6854423
35	0.995097	0.9999698	0.9999976	0.9968669	0.6854423
37	1.004008	1.00001	0.9999976	0.9968669	0.6854423
39	0.996732	0.9999919	0.9999976	0.9968669	0.6854423
41	1.002642	0.9999996	0.9999976	0.9968669	0.6854423
43	0.997868	0.9999964	0.9999976	0.9968669	0.6854423

Eq. (D12) is attractive because of its simplicity—easy to understand and easy to program—but it poses a potential problem. To ensure stability, it is necessary that

$$\frac{\Delta t\,\nu}{(\Delta y)^2} \le \frac{1}{2}.$$

Let's illustrate this using (D12). Choose ν=0.05 cm^2/s, Δy=0.1 cm, and Δt=0.12 s; of course, this guarantees that we're over the limit of ½. We'll put the calculation into a table and monitor the evolution of the nodal velocities.

Table D2. Explicit computation with unstable parametric choice(s).

t	i=1	i=2	i=3	i=4	i=5	i=6	i=7
0	1	0	0	0	0	0	0
Δt	1	0.6	0	0	0	0	0
2Δt	1	0.48	0.36	0	0	0	0
3Δt	1	0.72	0.216	0.216	0	0	0
3Δt	1	0.5856	0.5184	0.0864	0.1296	0	0
4Δt	1	0.7939	0.2995	0.3715	0.0259	0.0777	0
5Δt	1	0.6209	0.6394	0.1210	0.2644	0	0.0467
6Δt	1	0.8594	0.3173	0.5181	0.0197	0.1866	-0.0093
7Δt	1	0.6185	0.7630	0.0986	0.4189	-0.0311	0.1306

The problem we see immediately above is easy to resolve. We change our parametric choices to yield: $\frac{\Delta t \nu}{(\Delta y)^2} = 0.4$, and repeat the calculation.

Table D3. Explicit computation with stable parametric choice(s).

t	i=1	i=2	i=3	i=4	i=5	i=6	i=7
0	1	0	0	0	0	0	0
Δt	1	0.4	0	0	0	0	0
2Δt	1	0.48	0.16	0	0	0	0
3Δt	1	0.56	0.224	0.064	0	0	0
4Δt	1	0.6016	0.2944	0.1024	0.0256	0	0
5Δt	1	0.6381	0.3405	0.1485	0.0461	0.0102	0
6Δt	1	0.6638	0.3872	0.1843	0.0727	0.0205	0.0041
7Δt	1	0.6859	0.4158	0.2190	0.0965	0.0348	0.0090

This is an important lesson. If we need good spatial resolution, Δy will be small and Δt will need to be *very small*, perhaps prohibitively small. Fortunately, we do have options that will work well for this type of problem.

An Implicit Numerical Procedure

Consider a transient conduction problem with two spatial dimensions:

$$\frac{\partial T}{\partial t} = \alpha\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right]. \qquad \text{(D13)}$$

In this case, the stability requirement for an explicit solution is:

$\alpha \Delta t \left[\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} \right] \le \frac{1}{2}$, which can be prohibitive. However, there is an alternative.

The Peaceman-Rachford, or alternating direction implict (ADI) method can be especially effective for this type of parabolic partial differential equation. Let the indices i, j, and k represent x, y, and t, respectively. The first half of the ADI algorithm is used to advance to the k+1 time step:

$$\frac{T_{i,j,k+1} - T_{i,j,k}}{\alpha \Delta t} = \frac{T_{i+1,j,k+1} - 2T_{i,j,k+1} + T_{i-1,j,k+1}}{(\Delta x)^2} + \frac{T_{i,j+1,k} - 2T_{i,j,k} + T_{i,j-1,k}}{(\Delta y)^2}, \qquad \text{(D14)}$$

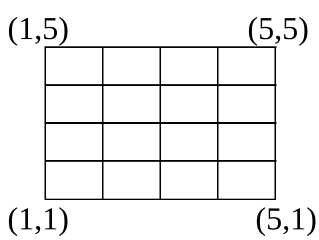
and the second half takes us to k+2:

$$\frac{T_{i,j,k+2} - T_{i,j,k+1}}{\alpha \Delta t} = \frac{T_{i+1,j,k+1} - 2T_{i,j,k+1} + T_{i-1,j,k+1}}{(\Delta x)^2} + \frac{T_{i,j+1,k+2} - 2T_{i,j,k+2} + T_{i,j-1,k+2}}{(\Delta y)^2}. \qquad \text{(D15)}$$

Note that neither step can be repeated unilaterally. Let’s look at a simple application. A two-dimensional slab of material is at a uniform initial temperature of 100°. At t=0, one face is instantaneously heated to 400°. Let Δx=Δy=1, as well as α=1 and Δt=1/8. We rewrite eq. (D14) isolating the k+1 terms on the right-hand side:

$$-T_{i,j+1,k} + \left(2 - \frac{(\Delta x)^2}{\alpha \Delta t}\right) T_{i,j,k} - T_{i,j-1,k} = T_{i+1,j,k+1} - \left(2 + \frac{(\Delta x)^2}{\alpha \Delta t}\right) T_{i,j,k+1} + T_{i-1,j,k+1}. \qquad \text{(D16)}$$

Now let’s illustrate the process with a simple square slab; the top, left, and right sides are all maintained at 100°. The bottom will be set to 400°. The nine interior nodes are initialized at 100°.



We apply (D16) at the interior points, row by row; the first horizontal sweep results in:

100	100	100
100	100	100
133.67	136.73	133.67

for the nine interior points. Now we recast (D15) for application to the columns in order to advance to the k+2 time step:

$$-T_{i+1,j,k+1}+\left(2-\frac{(\Delta x)^2}{\alpha\Delta t}\right)T_{i,j,k+1}-T_{i-1,j,k+1}=T_{i,j+1,k+2}-\left(2+\frac{(\Delta x)^2}{\alpha\Delta t}\right)T_{i,j,k+2}+T_{i,j-1,k+2}\,. \tag{D17}$$

We solve the simultaneous equations that result from applying this equation to the columns, and obtain:

100.55	100.6	100.55
105.5	106	105.5
154.42	159.37	154.42

If the total number of equations is modest, then a direct elimination scheme can be used for solution. The coefficient matrix follows the tridiagonal pattern (with 1, -10, 1, for the selected parameters), so the process is easy to automate. Smith (1965) notes that for rectangular regions the ADI method requires about 25 times less work than an explicit computation. Carrying out the procedure to t=1.75 yields:

114.91	120.25	114.91
146.35	161.01	146.35
221.06	247.42	221.06

for the interior nodes. Chung (2002) notes that this scheme is unconditionally stable which makes it very attractive for problems in which the time evolution is slow; i.e., we can employ a very large Δt relative to the elementary explicit technique.

1. Peaceman, D. W. and H. H. Rachford. The Numerical Solution of Parabolic and Elliptic Differential Equations, *Journal Soc. Indust. Appl. Math.* 3:28 (1955).

2. Smith, G. D. *Numerical Solution of Partial Differential Equations*, Oxford (1965).